

# REPORT DOCUMENTATION PAGE

AFRL-SR-AR-TR-03-

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1. REPORT DATE (DD-MM-YYYY) 02-07-2003		2. REPORT TYPE Final Technical Report		3. DATES COVERED (From - To) 9/1/1995 to 8/31/2002	
4. TITLE AND SUBTITLE FAST Center for Environmental Remediation, Fate and Transport Of Hazardous Chemicals				5a. CONTRACT NUMBER	
				5b. GRANT NUMBER F49620-95-1-0514	
				5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S) Vinayak N. Kabadi - Principal Investigator				5d. PROJECT NUMBER	
				5e. TASK NUMBER	
				5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)  North Carolina A&T State University, Greensboro, NC 27411				8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR, 4015 Wilson Blvd., Room 713, Arlington, VA 22203-1954				10. SPONSOR/MONITOR'S ACRONYM(S)	
				11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION / AVAILABILITY STATEMENT  Approve for Public Release: Distribution Unlimited					
13. SUPPLEMENTARY NOTES					
<b>20030731 040</b>					
14. ABSTRACT In 1995, U.S. Air Force Office of Scientific Research (AFOSR) funded an interdisciplinary research project entitled "FAST Center for Environmental Remediation, Fate and Transport of Hazardous Chemicals" at A&T with a funding of \$3.35 million for six years. The major accomplishments of the project include: (1) development of infrastructure and facilities for environmental research at A&T, (2) significant research contributions in environmental science and engineering, (3) graduation of 25 M.S. graduates in five different disciplines, (4) training of 16 undergraduate assistants, (5) publication of 12 refereed papers and numerous technical presentations and proceedings, (6) resulted in additional funding from NSF, EPA, DOE and USDA for environmental research, (7) initiation of a process to establish a State supported Center for Environmental Remediation and Pollution Prevention at A&T. Because of the FAST Center project, A&T will compete for funding and will make significant research contributions in environmental science and engineering.					
15. SUBJECT TERMS					
16. SECURITY CLASSIFICATION OF:  a. REPORT			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON Vinayak N. Kabadi
b. ABSTRACT					19b. TELEPHONE NUMBER (include area code) (336) 334-7564
c. THIS PAGE					

**AIR FORCE FAST CENTER FOR ENVIRONMENTAL  
REMEDIATION, FATE AND TRANSPORT OF HAZARDOUS  
CHEMICALS**

**Grant no. F49620-95-1-0514**

**FINAL TECHNICAL REPORT**

**Submitted to:**

**Air Force Office of Scientific Research (AFOSR)  
4015 Wilson Blvd., Room 713  
Arlington, VA 22203-1954**

**by**

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**July 1, 2003**

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## EXECUTIVE SUMMARY

Scientific research and technological development are critical for enhancing environmental quality, improving our nation's economy, and protecting the health of our citizens. The most challenging environmental issues facing society today range from local to regional and global, including sustainably using and managing our natural resources; maintaining biological diversity; maintaining a safe water resource; improving air quality; reducing exposure to toxic substances; limiting hazards from natural resources (e.g., geological and weather-related hazards), understanding climate change, and minimizing ozone depletion. Addressing these complex issues requires simultaneous efforts in a number of areas, such as, development of scientific tools, improved risk assessment techniques and new and more cost-effective environmental technologies. In recent years, there has been a general consensus amongst the federal government agencies that progress can be best made in this area by inter-disciplinary teams of researchers including scientists and engineers working collectively on various aspects of a single focused research problem (see, for example, "Strategic Planning Document", report from Committee on Environment and Natural Resources, CENR, National Science and Technology Council, NSTC, Whitehouse, Washington, D.C., 1996). Consequently, a number of recent solicitations for proposals in the area are for goal oriented research that requires large teams and inter-disciplinary work. To be competitive and contributive in this very important research area, academic institutions must develop organizational strategies that will promote the large research efforts discussed above.

In 1995, U.S. Air Force Office of Scientific Research (AFOSR) funded an interdisciplinary research project entitled "Air Force FAST Center for Environmental Remediation, Fate and Transport of Hazardous Chemicals" at A&T with a funding of \$3.35 million over six years. The project has been successful in developing facilities and research capabilities in environmental remediation at A&T. In 1996, A&T applied for and obtained the authorization to plan The Center for Environmental Remediation from the UNC General Administration. The research capabilities developed by our faculty have resulted in additional funding from Department of Defense, Department of Energy, Environmental Protection Agency, Department of Agriculture, and National Science Foundation. In 1999, NSF funded a four institution (UNC-CH, NC State, A&T, and UT-Austin) Science and Technology Center on Environmentally Responsible Solvents and Processes at the level of \$18 million for five years, with possible extension for another five years. A&T's funding is approximately \$2.2 million, and this project is being conducted in the FAST Center facilities.

During the first couple years of the project considerable efforts were expended in creating an infrastructure that would promote quality research. A very important part of this development was identification and renovation of laboratory space for the Center. The University allocated 3500 square feet of space for the FAST Center in the new IRC-Fort building. The space included four laboratories, a computer room, and an administrative office. The laboratories were remodeled with the installation of necessary benches, casework, fumehoods, plumbing and electrical services. They were fully operational from January 1, 1998. Major equipment were purchased for an analytical/processing laboratory, and a microbiology/radiochemical laboratory. These included a Hewlett-Packard gas chromatograph with mass spectrometric detector, a Hewlett-Packard liquid chromatograph, Packard Instruments scintillation counter, Mocrotox/Mutatox toxicity analyzer,

Sorvall centrifuge, Beckman spectrophotometer, Biolog microbial identification system, Millipore water purification system, respirometer.

The initial research thrusts were divided into three areas: (1) Biological remediation methods, (2) Chemical remediation methods, and (3) Fate and transport modeling. During the first year of the Center, although significant projects were initiated in the three areas, there was limited interaction between projects within an area, and hardly any interaction between the three areas in the research program. On October 10, 1996, a four-men team from Air Force that included Capt. Mike Chipley from AFOSR, Drs. Tom Stauffer and Jim Spain from Armstrong Laboratory at the Tyndall AFB, and Lt. Ita Udo-Aka from Wright-Patterson AFB, visited A&T to review the progress and determine the research direction for the FAST Center project. During the meeting, Capt. Chipley discussed two research problems of interest to Air Force, both related to the contamination because of deicing and icing inhibitor materials. The first problem involved laboratory characterization and degradability studies of new materials for potential deicing applications by the Air Force. These materials were synthesized at George Mason University. Samples of three of these materials were made available. The second problem involved site characterization and biodegradability studies of sites contaminated by propylene glycol based deicing materials at the Pope and the Seymour Johnson Air Force Bases. Capt. Chipley suggested that the FAST Center develop a research program in environmental impact studies of these deicing materials, and all new materials with potential site applications. Accordingly, a number of research projects were initiated addressing the problem of remediation and degradation of existing and new deicing materials. Identification of common materials also provided significant interactions between investigators and research projects.

In 1998, Air Force made a policy decision to withdraw from fundamental research in environmental science and engineering. This was quite a setback for the FAST Center project. The Armstrong laboratory at the Tyndall AFB was reorganized, and because of their new focus there was no room for continued interactions between them and the FAST Center. Nevertheless, the FAST Center investigators continued their research projects, and have made significant progress and contributions resulting in numerous publications, training of numerous graduate and undergraduate students, and soliciting additional funding for research from such agencies as NSF, EPA, USDA, DOE, etc. A number of these newly funded projects continue to utilize the FAST Center facilities. A major accomplishment of the FAST Center project has been the development of the infrastructure and the facilities to allow the initiation of a process to establish a State supported Center for environmental remediation and pollution prevention at A&T. It is expected that such a Center will be implemented shortly, and will coordinate all environmental research activities at A&T utilizing the facilities developed with the FAST Center funding.

## **GOALS AND OBJECTIVES**

1. The main objective of the FAST Center has been to promote cutting edge research on science and technology leading to new and improved remediation techniques necessary to address a number of difficult environmental problems facing the State of North Carolina and the Nation as a whole. The research efforts may be divided into the following categories:
  - (a) Development of new techniques for assessing the potential environmental risks associated with the use of various hazardous materials.
  - (b) Development of affordable techniques to prevent pollution by detoxifying waste streams prior to release to the environment.
  - (c) Development of new techniques for remediating contaminated sites
  - (d) Development of scaleup techniques for the design of field scale processes based on small scale studies.
  - (e) Development of experimental techniques and mathematical models to understand fate and transport of hazardous materials underground.
  - (f) Combine the chemical and bioremediation methods with the understanding of the fate and transport of hazardous chemicals to design in situ remediation technologies for selected contaminated sites.
2. To provide state-of-the-art analytical, process and computational support facilities to faculty members actively pursuing research in the area of environmental remediation.
3. To provide an organizational structure and teamwork necessary to compete for and accomplish large inter-disciplinary projects necessary to address many existing environmental problems.
4. To maintain a competitive and active Center that will sustain the research activities well beyond the proposed period of the FAST Center research project.
5. To strengthen the environmental component of the academic curricula of various departments across the A&T campus. This will include improvement of existing courses and introduction of new courses in the areas of strong research involvement of the Center.
6. To provide valuable experience and training to graduate and undergraduate students by involving them in research in the area of environmental science and technology .
7. To establish collaborative interactions with scientists on a national and international levels.

8. To establish cooperative and collaborative interactions with environmental industry in the State of North Carolina, neighboring states and some prominent companies across the Nation.
9. To conduct seminars and workshops that will promote interactions between A&T faculty and students and scientists from prominent research organizations.
10. To serve the local community by promoting outreach programs, and faculty interactions with local colleges, and high schools.

## **ORGANIZATION AND PERSONNEL**

FAST Center is a multi-disciplinary research center with contributions from faculty members from various departments. The Center has been headed by Dr. Vinayak N. Kabadi who has served as the Center Director. The following is the list of the core group of faculty who make up the Executive/Management Committee of the Center. These are also the co-principal investigators in the FAST Center project.

Dr. Vinayak N. Kabadi, Professor of Chemical Engineering, Center Director  
Dr. Shou-Yuh Chang, Professor of Civil Engineering  
Dr. Keith A. Schimmel, Associate Professor of Chemical Engineering  
Dr. Yusuf G. Adewuyi, Professor of Chemical Engineering  
Dr. G. B. Reddy, Professor and Chairman of Natural Resources and Environmental Design  
Dr. David Klett, Professor of Mechanical Engineering  
Dr. Thomas Jordan, Associate Professor, Biology Department  
Dr. Emmanuel Nzewi, Associate Professor of Civil Engineering

The Center has a dual accountability, and reports to the Dean of the College of Engineering, and the Vice-Chancellor for Research. The Center has also established interactions with a number of external organizations as listed below.

NSF-STC Center for Environmentally Responsible Solvents and Processes, UNC-Chapel Hill, and NC State.  
Air Force Research Laboratory, Wright-Patterson AFB  
Micell Technologies, Inc.  
Ecoflow, Inc.  
Procter & Gamble, Greensboro

A number of faculty members and their students conduct research in the CERPP facilities. The faculty, some recent graduate students, and undergraduate research assistants are listed below.

**Faculty Investigators:**

Dr. Yusuf G. Adewuyi, Chemical Engineering, E-mail: [adewuyi@ncat.edu](mailto:adewuyi@ncat.edu)

Dr. Shou-Yuh Chang, Civil Engineering, E-mail: [chang@ncat.edu](mailto:chang@ncat.edu)

Dr. Thomas Jordan, Biology Department, E-mail: [jordant@ncat.edu](mailto:jordant@ncat.edu)

Dr. Vinayak N. Kabadi, Chemical Engineering, E-mail: [kabadi@ncat.edu](mailto:kabadi@ncat.edu)

Dr. David Klett, Mechanical Engineering, E-mail: [klett@ncat.edu](mailto:klett@ncat.edu)

Dr. Emmanuel Nzewi, Civil Engineering, E-mail: [nzewi@ncat.edu](mailto:nzewi@ncat.edu)

Dr. G. B. Reddy, Natural Resources and Environmental Design, E-mail: [reddy@ncat.edu](mailto:reddy@ncat.edu)

Dr. Keith Schimmel, Chemical Engineering, E-mail: [schimmel@ncat.edu](mailto:schimmel@ncat.edu)

**Research Associates:**

Dr. Chao Ghao (1996-1997)

Dr. Lisa Carmichael (1998-1999)

Dr. Nasrollah Hamidi (1999, 2000)

Dr. Jehangir Imrani (1999)

Mr. Brian Westwood (2000- 2002)

**Graduate students with thesis titles and graduation dates:**

An Jin, "An Optimal Estimation Scheme for Subsurface Contaminant Transport Model Using Kalman-Bucy Filter", MS, December 1996.

Subhraj Jonnalagedda, "New Developments in Subsurface Contaminant Transport Models", MS, Unfinished.

Rhea Powell, "Laboratory Scale Experiments to Determine the Effect of Resistive Heating on Soil Microbial Communities", MS, December 1999.

Xin Cheng, "Kalman Filter Scheme for the 3-D Subsurface Transport Simulation with a Continuous Input", MS, December, 2000

Hong Guan, "First Order Uncertainty Analysis of DO – Neuse River, NC Case Study", December, 2000.

Asif Quader, "Determination of Diffusion and Resuspension Rate of Mercury by a Laboratory Study", August, 2001.

Duncan Ngari, "A comparison of GMS-MODFLOW and MSTS Models," MS, 5/15/1999

Bryan K. Alston, "A Predictive Model for the Optimal Selection of Non Point Source Urban Stormwater Best Management Practices," MS, 5/15/1999.

Wen Chen, "A Penalty-Based Model for the Optimal Operation of Multi-Purpose Multi-Reservoir Systems Using Dynamic Programming," 08/10/1997 (Partially supported by FAST Center)

Michelle R. Mims, "Mycological Potentials for Trichloroethylene Remediation", M. S., 5/1999

Sudheandra Mallya, "Fate of Tetrachloroethene in Piedmont soils", M. S., 12/2001

Pavithra Jayaraman, Comparative Study of Biodegradabilities of Fuel System Icing Inhibitors, M.S., 8/17/98.

Vinod Narayanan, Lab-Scale Modeling of the Effect of Resistive Heating Remediation Technologies on the Dynamics and Activity of Subsurface Microorganisms, M.S., 7/13/99.

Bhama Bhat, Biodegradation of an Aviation Fuel System Containing Icing Inhibitors, M.S., 12/01/00.

Samuel O. Owusu, "Simultaneous Absorption and Oxidation of NO<sub>x</sub> and SO<sub>2</sub> by Chemical and Sonochemical Methods", M.S. Thesis, August 2001.

Collins Appaw, "Sonochemical Reaction Kinetics of Carbon Disulfide Oxidation in Aqueous Solutions", M.S. Thesis, August 2000.

Riyad Jadalla, "Gas Stripping of Organic Pollutants and Detoxification by UV-Catalysis", M.S., Unfinished.

Vicky L. Harrison, "Gas Stripping of Organic Pollutants using a Shallow-tray Stripper and Detoxification by UV-catalyzed Photolysis, M.S. Thesis, August, 1997.

David Williams, "Photocatalytic Degradation of Organics in Aqueous Media", M.S., May, 1998.

Kwame Hammond, "Partition Coefficient Measurement by the Slow-Stirring Method", M.S., May, 1999.

Shahnaj Begum, "Supported TiO<sub>2</sub> Catalyst for Photocatalytic Detoxification", M.S., May, 2000.

Anand Javvadi, "Partitioning of Higher Alcohols in Alkane – Water at Dilute Concentrations", M.S., December, 2000.

Parag Adhangale, "Molecular Dynamics Computer Simulation of the Air-Water Interface", M.S., July, 2001.

Derrick McCrae, "Supported TiO<sub>2</sub> Catalyst for Solar Detoxification", M.S., August, 2002.

Dexter McQueen, "Isolation and Growth of Glycol Degrading Bacteria", M.S., August, 2000.

**Undergraduate research assistants:**

Tomeka Terry, "Assessment of Soil Toxicity Using the Microtox ® System, Lab Scale Modeling of Resistive Heating Remediation Technologies", 8/97 – 12/98.

Charla Gaskins, "Research on Creosote Wastes Through Technical Collaboration with the US Army Corps of Engineers, Waterways Experiment Station", 6/98 – 5/99.

Damien Thomas, "Development of PC-Workstation Cluster for Groundwater Modeling," 5/14/1996 to 6/30/1996

Jonathan Brown, "A Comparative Implementation of MODFLOW and MSTS," 8/1996 to 12/1996

Kaisha Homan, Comparative Study of Biodegradabilities of Fuel System Icing Inhibitors, Fall 1996.

Caroline Medley, Determination of Biodegradation Rate of Petroleum-Contaminated Sludge and Soil Using an Oxygen Respirometer, 1995-96.

Archie Alston, Design of Gas-Liquid Contactors, Spring, 2000

Keisha Brown, Catalytic NO<sub>x</sub> Removal, Spring, 1995

Jonathan James, NO<sub>x</sub> Absorption and Oxidation, Fall, 1995

Kimberly Wingfield, TCE Oxidation by Fenton's Reagent, Spring, 1996

Cassandra Burch, TCE Oxidation by Fenton's Reagent, Fall, 1997

Adrienne Hall, Low-profile Stripping of Organic Pollutants, Spring, 1997

Stacey Goins, Low-profile Stripping/Photolysis of TCE, Fall, 1996

Christy Walker, Low-profile Stripping/Photolysis of MTBE, Spring, 1996

Shahera Walker, Partition coefficients of organic pollutants, 1999-2000

Terrence Bekoe, VLE of systems containing carbon dioxide, 2000-2001

## **FACILITIES**

The University allocated 3500 sq. ft. of space for the FAST Center project which was renovated into environmental laboratories. These laboratories will constitute the core space for environmental research at A&T for quite some time in the future. The space is divided into four laboratories: a radiochemical/microbiology laboratory, an analytical laboratory, and two processing laboratories. Additionally, the Center also has an administrative office, and a computational laboratory. The major equipment available in the laboratories are listed below:

### **Computational:**

- Compaq- Alpha UNIX Workstation
- HP 9000 workstations (2)
- IBM-Pentium PCs (4)
- Peripherals

### **Analytical:**

- HP 6890 GC/MS system
- HP Liquid Chromatographic system
- HP 6890 GC
- Liquid scintillation counter
- Spectrophotometers
- Perkin-Elmer Thermogravimetric analyzer
- Perkin-Elmer elemental analyzer

### **Microbiology/ Biodegradation:**

- Microtox/Mutatox toxicity analyzer
- Microbial identification system (Biolog)
- 24-station AER-200 Respirometer
- Bioflo III fermentor vessel assembly
- Benchtop shell freezer
- Benchtop sterilizer/dryer

### **Processing:**

- Shallow tray air stripper
- Photocatalytic reactors
- Cryogenic and environmental chambers (2)
- Cryogenic isothermal calorimeter (CSC, Inc.)
- Cryogenic differential scanning calorimeter (CSC, Inc.)

## **OTHER GRANTS**

A number of other grants for environmental research have complemented the FAST Center activities. Some of these grants are listed below.

Uzochukwu, G. A. (PI), Kabadi, V. N., Ilias, S., Adewuyi, Y. G., Roberts, K. (Co-PIs), "NSF-STC Center for Environmentally Responsible Solvents and Processes," Sub-Contract from UNC-CH NSF-

STC Center (J. DeSimone, R. Carbonnel, Directors), National Science Foundation, \$2.2 million, 1999-2004.

Chang, S.-Y. (PI), Nzewi, E., Roberts, K.L. and Reyes, M., "Interdisciplinary Environmental Engineering Fellowship Program for Agricultural, Chemical and Civil Engineering," GAANN-U.S. Department of Education, \$380,625, 8/1/2000 – 7/31/2003.

Kemp-Glass, M., Schimmel, K.A., et al., "Enhancing Biotechnology Capabilities at North Carolina A&T State University," North Carolina Biotechnology Center, \$170,000, 10/01 to 10/02.

Ilias, S., Schimmel, K.A., King, F., "International Development Partnership with Bangladesh University of Engineering & Technology (BUET) to Develop Collaborative Research in Pollution Prevention," UNCF/International Development Partnerships Activity, \$254,603, 5/01 to 4/03.

Reddy G. B. (Co-PI). "Integrated Crop and Sylvan Systems with Swine": A state and National initiativeUSDA-SARE, University of Georgia. 1999-2001 , \$156,262

Reddy G. B. (PI). "Swine Wastewater Treatment by Using constructed Wetlands". USDA/CSREES, Evans-Allen: 1998-2001, \$330,000

Nzewi, E. U. (PI), Yu, Anna (Co-PI), and Perkins (Co-Investigator), "Design and Implementation of a Web-Based GIS Road Closure Information System," US Department of Transportation, Federal Highway Administration, Office of Acquisition Management, \$215,000, 8/2000 to 9/2002.

Nzewi, E.U. (Co-PI) and Reddy M. R. (PI), " Using Spatial Statistics to Teach GIS/GPS and Enhance Problem-Solving Skills, " US Department of Agriculture, \$200,000, 10/2000 to 9/2001.

Schimmel, K. A. (PI), and Carmichael, L. M., "The Effect of Soil Resistive Heating on the Activity and Population Dynamics of Subsurface Microorganisms," Brooks AFB, \$99,000, 9/1997 to 12/1998.

## **PUBLICATIONS**

### **Refereed papers:**

Jin, A., and S.-Y. Chang, "Field Estimation of Standard Deviations for a 3-D Gaussian Model," J. of Environmental Engineering, ASCE, 122 (7), July 1996.

S.Y. Chang, X. Chen, and A. Jin "Kalman-Bucy Scheme for Subsurface Contaminant Transport Models," Journal Ground Water (under revision).

Reddy, G.B.; Hunt, P.; Philips, D.; Stone, K.; Grubbs, A. Treatment of Swine Wastewater in Marsh-Pond-Marsh Constructed Wetlands. *Journal of Water Science & Technology*. 2001, (In Press).

Bhat, B., Schimmel, K.A., Jayaraman, P., "Interaction Effects during the Biodegradation of Fuel System Icing Inhibitors," Journal of Bioremediation, (In Press).

Jayaraman, V., Mahgnani, Y., Schimmel, K.A., Carmichael, L., "Modelling of Lab-Scale Resistive Heating Effect on Soil Microbial Communities," Journal of Bioremediation. (In review)

Adewuyi, Y.G. Sonochemistry: Environmental Science and Engineering Applications. Industrial & Engineering Chemistry Research, 40, 4681, 2001.

Adewuyi, Y.G.; He, X.; Shaw, H.; Lolertpihop, W. Simultaneous Absorption and Oxidation of NO and SO<sub>2</sub> by Aqueous Solutions of Sodium Chlorite. Chemical Engineering Communications, 1999, 174, 21-51.

Adewuyi, Y.G.; Harrison, V.L.; Jadalla, R.A. Low-Profile Stripping of Organic Pollutants and Destruction by Gas-Phase Photolysis". In: Physical, Chemical and Thermal Technologies: Remediation of Chlorinated and Recalcitrant Compounds, G.B. Wickramanayake and R.E. Hinche (editors), Battelle Press, Columbus, 467-472, 1998.

Adewuyi, Y.G. and Appaw, C. "Sonochemical Oxidation of Carbon Disulfide in Aqueous Solutions: Reaction Kinetics and Pathways," Ind. Eng. Chem. Research, 41, 4957, 2002.

Adewuyi, Y.G.; He, X.; Appaw, C; Shaw, H. Absorption and Oxidation of NO<sub>x</sub> with Aqueous Solutions of NaClO<sub>2</sub> in a Venturi Scrubber in the Presence and Absence of SO<sub>2</sub>. Chemical Engineering Communications, (In Review).

Begum, S.; Williams, D.; Kabadi, V. N. "Supported TiO<sub>2</sub> Catalyst for Photocatalytic Detoxification", Environmental Science & Technology, in Review.

Javvadi, A.; Kabadi, V. N. "Partition Coefficients and Ternary Diagrams of environmental Significance", Industrial and Engineering Chemistry Research, in Review.

#### **Proceedings and presentations:**

Uzochukwu, G.A., Reddy, G.B., Editors, Environmental Remediation Science and Technology, Proceedings of the 1998 National Conference, Battelle Press, Columbus, 1999.

Jin, A., and S.-Y. Chang, "An Optimal Estimation Scheme for Subsurface Contaminant Transport Model Using Kalman-Bucy Filter," Proc. the Joint USAF/ARMY Contractor/Grantee Meeting, Panama City, FL, January 14-17, 1997.

Chang, S. Y., "Optimal Estimation Scheme in Subsurface Contaminant Transport," Proc. 6<sup>th</sup> Mainland-Taiwan Environmental Protection Conference, Kaoshiung, Taiwan, December 7-11, 1999.

Morton, B., and S. Y. Chang, "Generating Low Level Mixed Waste Management Alternatives", Proc. Waste Management '99 Conference, Tucson, AZ, March 1-4, 1999.

S. Y. Chang and H. Guan, "First Order Uncertainty Analysis of DO", Proc. The Seventh Mainland-Taiwan Environmental Protection Academic Conference, Wuhan, China, April 20-24, 2001.

S. Begum, D. Williams, V.N. Kabadi, "Supported TiO<sub>2</sub> Catalyst for Photocatalytic Degradation of Organic Pollutants", presented at the National Conference on Environmental Remediation Science and Technology, Greensboro, North Carolina, September 8-10, 1998.

K. Hammond, V.N. Kabadi, "Partition Coefficients of Organic Pollutants between Aqueous and Non-Aqueous Phases", presented at the National Conference on Environmental Remediation Science and Technology", Greensboro, North Carolina, September 8-10, 1998.

P. Adhangale, V.N. Kabadi, "Molecular Dynamics Computer Simulations of Partition Coefficients of Organic Molecules at the Air-Water Interface", presented at the Annual AIChE Meeting, Miami Beach, Florida, November, 1998.

V.N. Kabadi, "MD Simulations of Phenomena at the Oil-Water Interface", presented at the Symposium in Honor of Dr. Eli Ruckenstein, AIChE Annual Meeting, Dallas, Texas, November, 1999.

V.N. Kabadi, B. M. Westwood, "A Novel Pycnometer for Measurement of Volumes of Mixing at High Temperatures", presented at the AIChE Annual Meeting, Los Angeles, California, November, 2000.

V.N. Kabadi, A. Javvadi, "Partition Coefficients of Higher Alcohols in Water-Alkane Systems", presented at the Annual AIChE Meeting, Los Angeles, California, November, 2000.

Nzewi, Emmanuel U, "A Comparative Implementation of MODFLOW and MSTS," Proceedings MODFLOW-98 Conference, Golden, CO, October 4-8, 1998

Nzewi, E. U., G. A. Uzochukwu and H. E. Nwankwo, "Development of a Relational Database for Remediation Technologies, *Proceedings*, National Conference on Environmental Remediation, Greensboro, Battelle Press, July, 1999.

Nzewi, E. U. and Wen Chen, "Development of an Operations Model for a Multi Reservoir System Using Dynamic Programming: Computational Issues," presented at the 24th Annual ASCE Water Resources Planning and Management Conference, in Houston, TX, April 5-9, 1997.

Nzewi, E. U. and D. Ngari, "Development of PC-Workstation Cluster for Groundwater Modeling," *Proceedings*, National Conference on Environmental Remediation, Greensboro, Battelle, Press, July, 1999.

Nwankwo, H. E, E. U. Nzewi and G. A. Uzochukwu, "A User-Centered Database System for Assessment and Evaluation of Environmental Restoration Technologies," *Proceedings*, National Conference on Environmental Remediation, Greensboro, Battelle, Press, July, 1999.

Nzewi, Emmanuel U and B. K. Alston, "A Model for the Selection of Cost-Effective Non-Point Source Urban Stormwater Best Management Practices," presented at the session on Water Resources Engineering, 1999 ASCE North Carolina Section Spring Workshops, Charlotte, NC, May 04, 1999

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Nzewi, Emmanuel U and Ademola A Onafuye, "An Investigative Approach to Site Remediation," *Proceedings*, 2001 World Water & Environmental Resources Congress, Orlando, FL, May 19 – 24, 2001

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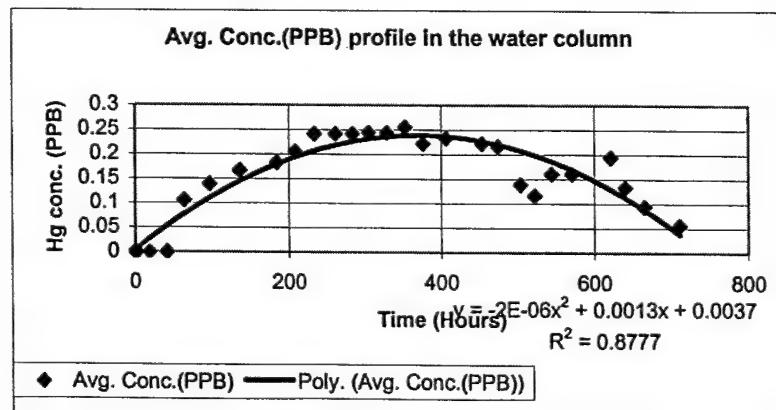
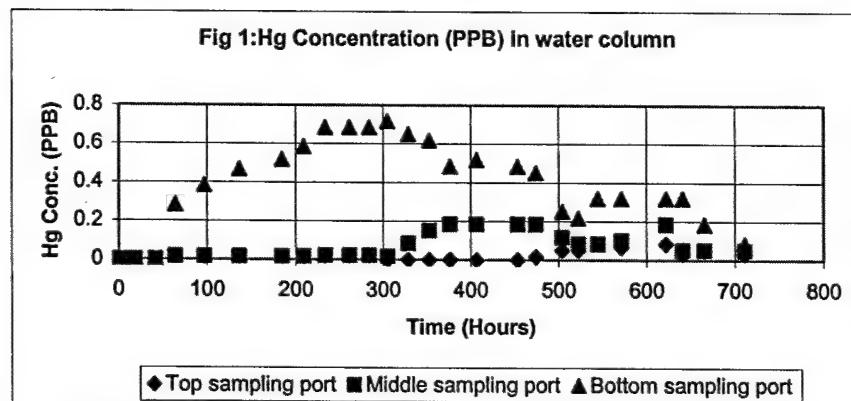
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## **PROJECT SUMMARIES**

In what follows, we present short one page summaries of some current research projects in CERPP.

**Project Title:** Determination of Diffusion and Resuspension Rate of Mercury by a Laboratory Study  
**Investigator(s):** Dr. S-Y Chang  
**Student(s):** Asif Quader

**Summary:** The estimation of diffusion and resuspension rate of mercury is important for developing steady and unsteady state toxic substance models of lakes. In this study, we have performed a laboratory simulation of a lake. The sediment particles from Lake Townsend were homogeneously mixed with 10 ppb mercury standard and placed in the tank bottom. The mercury concentration of the water column was determined by the cold vapor atomic absorption spectrophotometry. Water samples were collected from three vertical sampling ports in the tank at 24-hour interval for a period of one month. The concentration profile in Fig 1 shows that the mercury gradually diffuses upward and its concentration starts to increase in the layer above the sediment column. The mercury concentration reaches a maximum value of 0.76 ppb in the water column right above the sediment layer. Indicating that only 7.6% of the total mercury remains in dissolved form and diffuses upward, the rest remains bound to the sediment particles. Fig 1 also shows that as the mercury concentration in the bottom layer starts to reduce, the mercury concentration in the middle layer starts to increase and it reaches a peak value of 0.18 ppb. Ultimately the whole water column reaches an equilibrium concentration. The average concentration profile (Fig 2) in the water column indicates that, initially the diffusion process is predominant, after a definite time it reaches an equilibrium phase and finally the heavy metal settles down in the lake bottom. Using the unsteady state concentration profile of the average mercury concentration in the water column, the diffusion rate of mercury was found as 0.021 cm/hr. The diffusion rate of mercury based on empirical equation was 0.0083 cm/hr. The small volume of water column may be responsible for the high diffusion rate of mercury. The same approach can be taken to calculate the resuspension rate of mercury in the laboratory simulation of lake.



**Project Title:** Assessment of Soil Toxicity Using the Microtox® System

**Investigator(s):** Lisa Carmichael

**Student(s):** Tomeka Terry, Damien Thomas

**Summary:** This project was initiated via conversations with the personnel of the Operational Toxicology Laboratory at Wright-Patterson Air Force Base. Major Gary D Meyer indicated that the Air Force was in the process of developing a toxicity test using the response of human cell lines to contaminated soils. This project has been titled "Toxicological Methods for Use In Operational Contingencies" by the Air Force. The test would be used to indicate dangers posed to Air Force Personnel by soils in bases and other sites around the world. The objectives of this project were to analyze soils supplied by the Air Force in the Microtox® and Mutatox™ assays.

Microtox® analyses were completed with 1) water exposed to hydrocarbon contaminated soils (supernatant studies) and 2) slurries of contaminated soil /water. The soils were provided by Wright-Patterson Air Force Base (IC, IT, AC, AT, EC, ET). The mutagenicity of the three contaminated soils (IT, AT, ET) was tested with the Mutatox™ system following the basic Mutatox™ protocol. Microtox® analysis of the soils indicated that extracts of the AC, IC, and EC soils were not toxic (Table 1). These were later identified as control uncontaminated soils. Of the remaining soils, the ET and AT soils were similar in their toxicity while the IT soil was much less toxic than the others. When the slurries were tested, however, they were an order of magnitude more toxic than the water extracts. As with the extracts, the AT and ET soil slurries were similar in toxicity but the IT soil was found to be much more toxic than the other soils. In order to account for the light quenching activities of the slurries, the uncontaminated soils were also tested but were found to have little effect on light production.

Results of the Mutatox™ tests demonstrated that water extracts of the soils were mutagenic but only after exposure to the rat liver S9 medium. The response to the extracts in the medium lacking rat liver S9 fraction was not different from that found in the unamended medium controls. With the exception of high responses from one of the AT soil dilutions, extracts of the contaminated soils yielded similar amounts of light production. The most concentrated dilutions usually do not have the largest mutagenic response due to the toxicity of the more concentrated dilutions (which will reduce light production). Light production in a benzo(a)pyrene (10µg/L) standard is included as a reference.

**Table 1. Results of the Microtox® Assay run on soil extracts and slurries.**

Test Type	Soil	EC <sub>50</sub> (95% Confidence Interval)
Supernatant	EC	NT
	AC	NT
	IC	NT
	ET	10.21% (4.28 - 24.39)
	AT	10.66% (5.68 - 19.99)
Slurry	IT	81.59% (28.68 - 232.12)
	EC	NT
	AC	NT
	IC	NT
	ET	1.405% (1.014 - 1.948)
	AT	1.385% (1.078 - 1.781)
	IT	0.04737% (0.04613 - 0.04865)
	IT*	0.05496% (0.04323 - 0.06987)

\* The It soil was tested with two different aliquotes of soil; NT= not toxic at concentration tested

**Project Title:** The Toxicity of Experimental Fuel Deicing Agents

**Investigator(s):** Lisa Carmichael

**Student(s):** Tomeka Terry, Damien Thomas

**Summary:** One of the projects undertaken by the FAST Center was to investigate the degradability and toxicity of experimental fuel deicing agents synthesized by Dr. George Mushrush of George Mason University. Three of the agents were identified by the Materials Division of Wright Patterson Air Force Base as candidates for use as deicing agents M1 (2,2-Dimethyl-1,3-Dioxolane-4-methanol), M2 (1,3-Dioxolane-4-Methanol) and M3 (2-Methyl-1,3-Dioxolane-4-Methanol). Microtox® analysis of the compounds indicated that M1 and M3 are similar in toxicity but are an order of magnitude more toxic than the M2 compound (Table 1). Mutatox™ analysis of the fuel deicers indicated that the materials were mutagenic with and without the rat liver S9 fraction (Table 2). Light production was highest, however, in the absence of the rat liver S9 fraction. Within each media incubation (with and without rat liver S9), light production by the fuel deicers was similar.

**Table 1. Results of the Microtox® analysis of experimental fuel deicers**

Deicing Agent	EC <sub>50</sub> *
M1	6.045 (4.398 – 8.307)
M2	37.30 (30.10 – 46.20)
M3	6.848 (5.431 – 8.634)

\*Concentration in mg/L and (standard deviation)

**Table 2. Mutatox™ analysis (light level readings) of three experimental fuel deicers (M1, M2, M3) in both a rat liver S9 medium and Mutatox™ medium.**

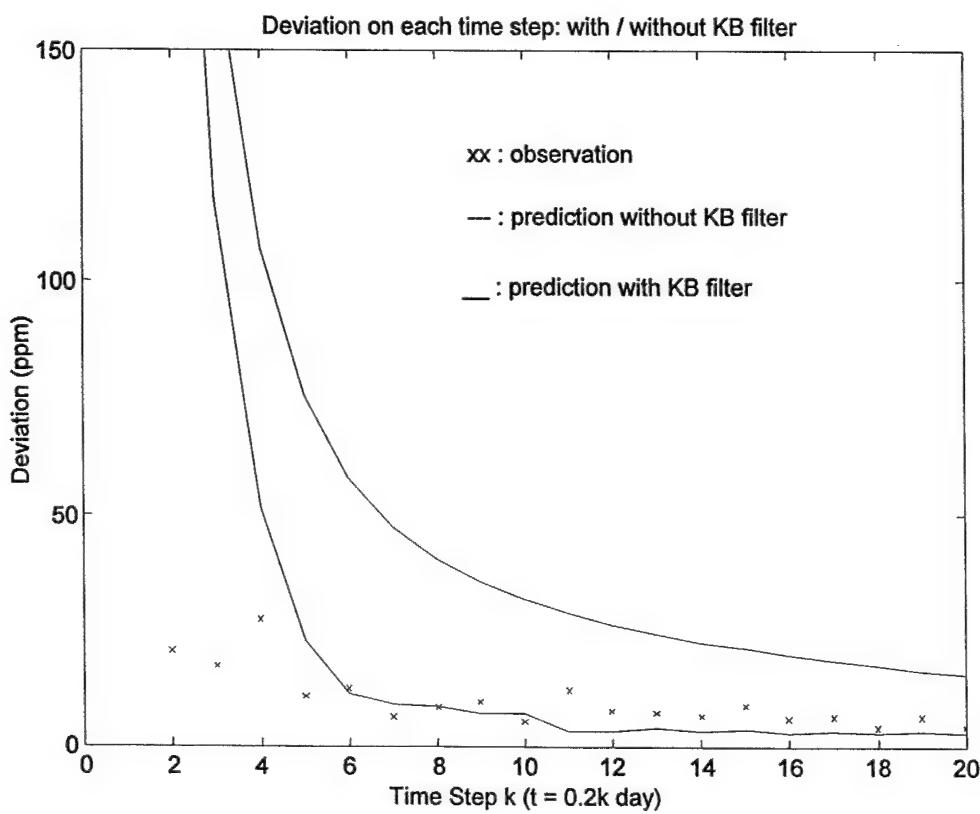
Fuel Deicer (mL/L)	S9 Medium			Mutatox™ Medium		
	M1	M2	M3	M1	M2	M3
0.046875	14	2	8			
0.09375	29	22	4			
0.1875	32	11	55			
0.375	58	51	21			
0.75	15	24	21	14	45	16
1.25	24	30	22	91	49	57
2.5	6	34	13	175	338	502
5	43	23	15	208	263	322
10	78	7	39	92	189	1
20	1	120	1	6	31	1

**Project Title:** Kalman-Bucy Scheme for Subsurface Contaminant Transport Models

**Investigator(s):** Shou-Yuh Chang

**Student(s):** An Jin and Xin Cheng

**Summary:** In the subsurface contaminant transport models, errors coming from the numerical model and the initial data field can cause unavoidable prediction deviations. Using the Kalman-Bucy (KB) filter to combine more relative information into model dynamics should be able to reduce this kind of deviation. To show the effectiveness of the KB scheme, a two and a three-dimensional Forward-Time and Central-Space (FTCS) advection-dispersion-adsorption subsurface transport models are described and constructed to predict the pollutant concentration of a contaminant plume with the error scale at 12 and 16 ppm respectively. The numerical random noise simulation schemes are designed to create "observation" data with error scale at 14 and 5 ppm respectively. Then the integrated KB filter schemes are constructed using Matlab routines and operated with the FTCS dynamics. The results from the implementation indicated that the prediction errors of the KB scheme, no matter in two or in three-dimensional prediction model, are much smaller than either that from the prediction FTCS scheme or that from the observation data. Furthermore, the results show that with combining the observation data dynamically in each time step, the KB schemes reduce the prediction error for a 60-80% reduction. Thus, results from this paper indicate that in the subsurface transport simulation field, the KB scheme can provide better prediction, which is much closer to the "true" values than the non-KB model does.



**Project Title:** Investigation of Natural Attenuation at DOE Site

**Investigator(s):** Emmanuel U. Nzewi, PhD, PE

**Student(s):** Ahmed Ademola Onafuye

**Summary:** *Monitored* Natural Attenuation (MNA) is a term that refers specifically to the use of or rather reliance upon natural attenuation processes as part of overall site remediation strategy. The term “monitored” is used to indicate that while attenuation is assumed, an active monitoring of the site is maintained to verify that natural processes continues to lead to the reduction of mass, toxicity, volume or concentration of the contaminants in soil or groundwater.

The use of MNA has been proposed at a US Department of Energy (DOE) site as a passive groundwater cleanup strategy to address the dilute fringes of the contaminant plume. In this study, the second line of evidence (i.e. documented loss of contaminant mass) will be used as a preliminary indicator of the feasibility of MNA as a remedial option for the fringes. Ten (10) years (1989-1999) of groundwater monitoring data from selected monitoring wells for the preliminary (first line of evidence) demonstration of natural attenuation of chlorinated aliphatic hydrocarbons (PCE, TCE) at the southern sector of the Administrative and Management Area (A/M) of the Savannah River Site Aiken, South Carolina.

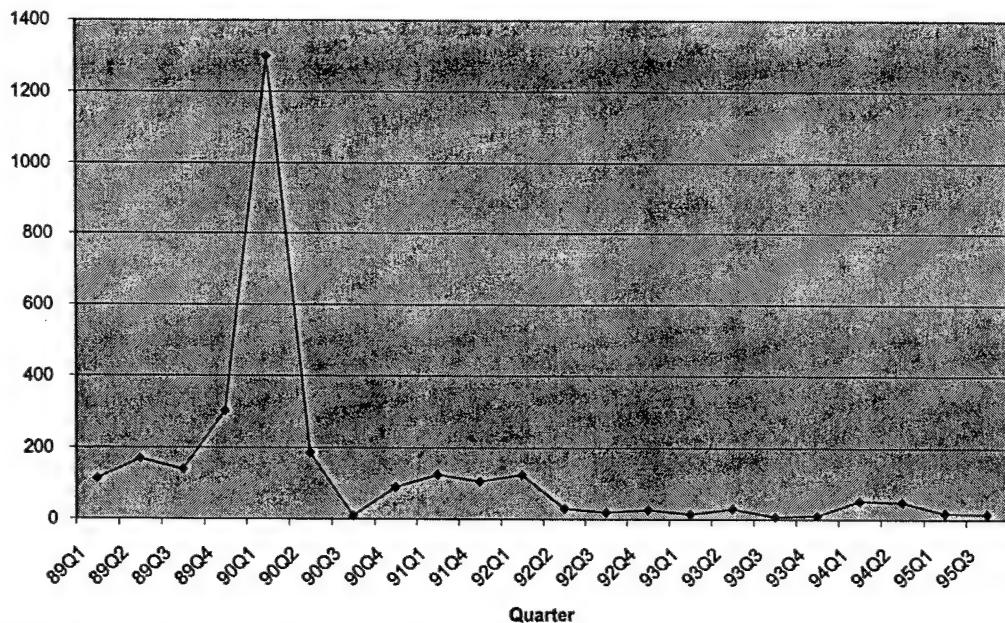
Natural Attenuation relies on natural processes (physical, chemical, and biological). These processes under favorable conditions will reduce the mass, toxicity, volume, or concentration of contaminants in soil or groundwater. These in-situ processes include biodegradation, dispersion, dilution, sorption, volatilization, and chemical or biological stabilization, transformation, or destruction of contaminants.

To support remediation by natural attenuation, it must be scientifically demonstrated that degradation of site contaminants is occurring at rates sufficient to be protective of human health and the environment. Three lines of evidence are admissible in the support of natural attenuation; they are

- Observed reduction in contaminant concentrations along the flow path down-gradient from the source of contamination.
- Documented loss of contaminant mass at the field scale using:
  - Chemical and geochemical analytical data (e.g., decreasing parent compound concentrations, increasing daughter compound concentrations, depletion of electron acceptors and donors, and increasing metabolic byproduct concentrations).
  - A conservative tracer and a rigorous estimate of residence time along the flow path to document contaminant mass reduction and to calculate biological decay rates at the field scale.
- Microbiological laboratory data that support the occurrence of biodegradation and give rates of biodegradation.

At a minimum, the investigator must obtain (confirm) the first two lines of evidence or the first and third lines of evidence. The sample trends, contour and area plots shown below are used to support the first two lines of evidence for this DOE SRS study.

### Lower Lost Lake: Well #MSB-38B for TCE



### Variation of TCE Concentration by Quarter at Monitoring Well MSB-38B



DCE Concentration in 1992Q2 over the SRS A/M Area

Lwrlspce2\_all : 88.400

712.00316018

655.112264

598.221367

541.330471

484.439574

427.548678

370.657782

313.766885

256.875989

199.985092

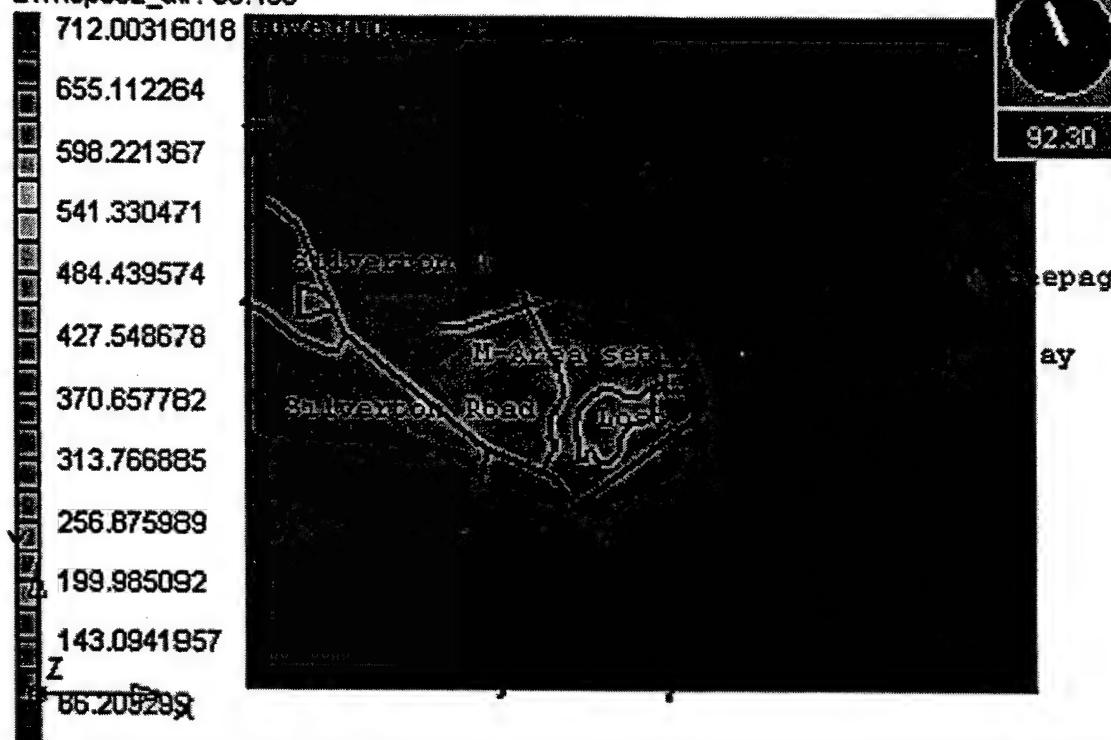
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Z

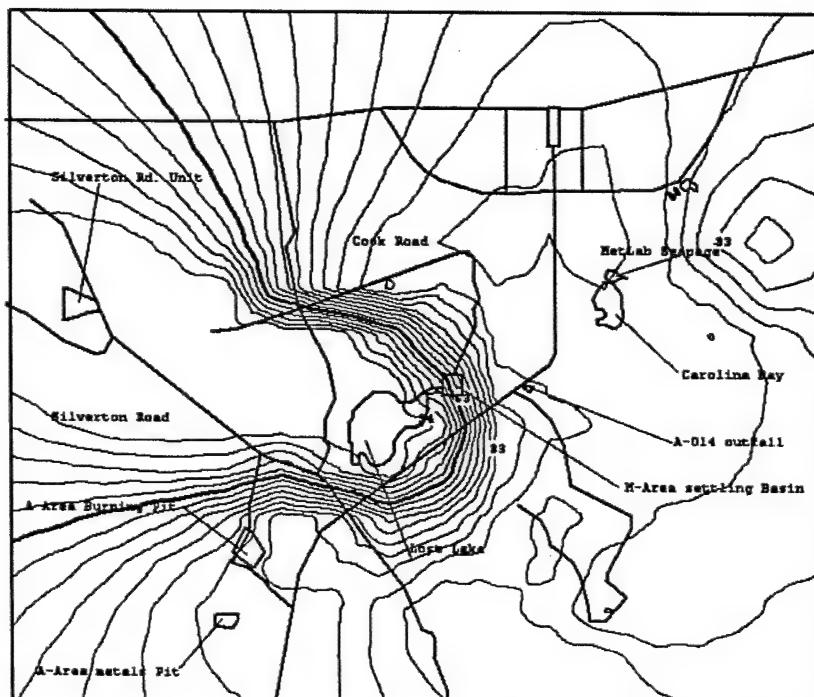
86.209295



92.30



PCE Concentration in 1992Q3 over the SRS A/M Area



PCE Concentration Contours in 1992Q3 over the SRS A/M Area

**Project Title:** Determination of the Liquid/Soil Equilibrium Constant of Tetrachloroethene in Enon Soil  
**Investigator(s):** G. B. Reddy

**Objective:** To determine the equilibrium constant between the liquid and Enon soil for Tetrachloroethene (PCE)

A series of experiments were carried out to optimize the experimental conditions for kinetic determinations of the environmental fate of PCE in Enon soil. Transport processes within a particular soil and between other parts of the ecosystem, such as the air and water, are necessary to anticipate the effect of PCE to our environment. Eight-day experiments were conducted in which a solution of aqueous PCE was placed in a system of Enon soil. The approach to equilibrium between the water and soil was monitored by determining the aqueous PCE concentration for a span of 8 days. (Figure A) For the physical processes

$PCE(aq) \Rightarrow PCE(soil)$      $d[PCE(aq)]/dt = a[PCE(aq)]$   
and     $PCE(soil) \Rightarrow PCE(aq)$      $d[PCE(soil)]/dt = b[PCE(soil)]$   
the equation for the approach to the equilibrium [  $PCE(aq) \leftrightarrow PCE(soil)$  ] is

$$[PCE(aq)] = ((b+a \cdot e^{-(a+b)t})/(a+b)) \cdot [PCE(aq)]_0$$

This curve was fit to determine the two rate constants (a and b) for the equilibrium constant determination (a/b). The curve-fitting routine was at the web-site of John C. Pezzullo who is a Associate Professor in the Departments of Pharmacology and Biostatistics at Georgetown University, in Washington, DC. His statistics are java-driven and can be done interactively in his pages. The experimental versus statistical decay curves are in Figure A.

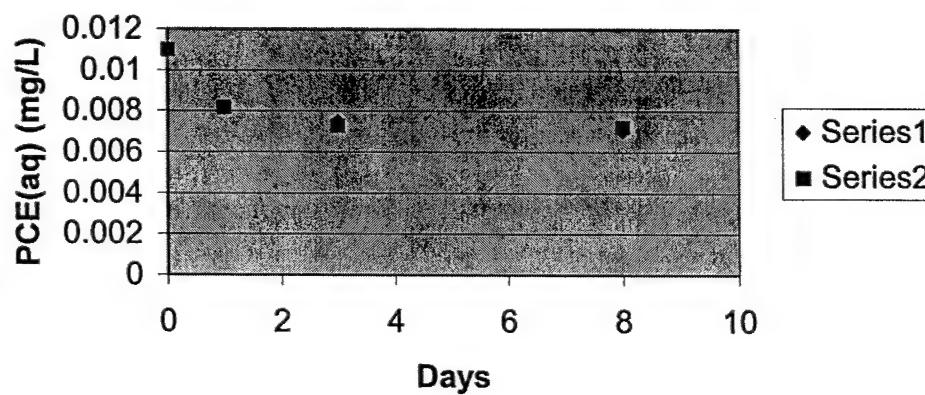
Corr. Coeff. = 0.996237;  $r^*r = 0.992487$ ; RMS Error = 0.000188

Parameter Estimates...

$a = 0.467655 \pm 0.071751$      $b = 0.898006 \pm 0.166082$      $a/b = 0.52077$

This equilibrium constant of the liquid/soil system is 0.52077.

**Figure A: PCE APPROACH TO EQUILIBRIUM IN ENON SOIL**



**Project Title:** White Rot Fungal Remediation of Tetrachloroethene in Aqueous Solution  
**Investigator(s):** G. B. Reddy

**Objective:** To determine whether or not Tetrachloroethene (PCE) could be metabolized by White Rot Fungi (WRF) in the presence and absence of growth media.

Two experiments were performed:

1. Ten mL of sterile water and 100  $\mu$ L of growth media and PCE was innoculated with WRF. The control for this experiment was a system with no WRF in the system. PCE incurred approximately an eight percent remediation by WRF with no media present. (Table 1)
2. Ten milliliters (mL) of sterile water and varying amounts of growth media was placed into a 22 mL, crimp-sealed vial with teflon lined septa. Half of the containers were innoculated with a small plug of WRF. PCE incurred approximately a forty percent remediation by WRF with media present. (Table 1, Figure A)

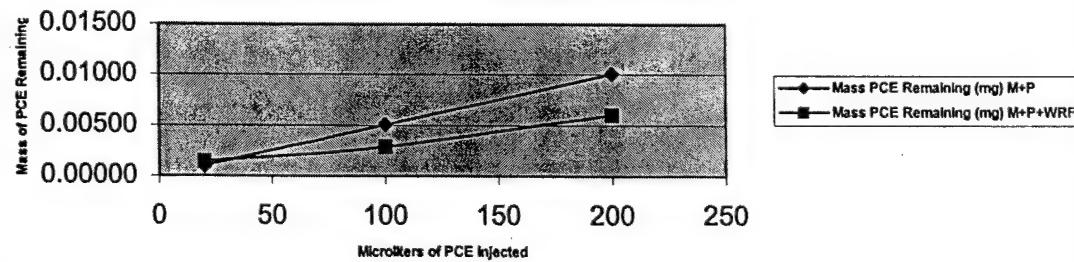
Three conclusions can be drawn from this work:

- a. PCE is metabolized by WRF. (Table 1, Figure A)
- b. Media is not necessary for the remediation of PCE by WRF. (Table 1)
- c. PCE consumption by WRF is increased approximately five-fold with the addition of growth media to the system. (Table 1)

TABLE 1

SAMPLE ID	Mass of PCE in System (mg)	Percent Remediation
10ml H <sub>2</sub> O + 100 ul PCE	0.01159	7.98
10ml H <sub>2</sub> O + 100 ul PCE + WRF	0.01067	
10ml Media + 200ul PCE	0.00985	38.39
10ml Media + 200ul PCE +WRF	0.00607	
10ml Media + 100ul PCE	0.00450	44.09
10ml Media + 100ul PCE + WRF	0.00251	
10ml Media + 20ul PCE	0.00053	-87.20
10ml Media + 20ul PCE + WRF	0.00099	

Figure A: WRF Degradation of PCE

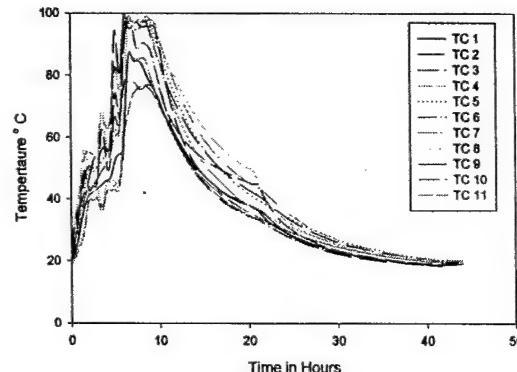
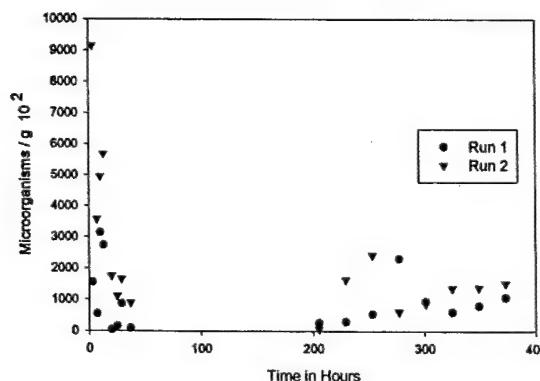


**Project Title:** Lab-Scale Modeling of the Effect of Resistive Heating Remediation Technologies on the Dynamics and Activity of Subsurface Microorganisms

**Investigator(s):** Keith Schimmel

**Student(s):** Vinod Narayanan, Rhea Powell-Jones

**Summary:** Resistive heating of soils is a heating method in which electrodes are placed in a contaminated site and increase the subsurface temperature to over 100° C. Under this high temperature the target contaminants are solubilized and oxidized. It has been successfully used for the in situ remediation of contaminated sub-surface sites that have a large fraction of dense non-aqueous phase liquids (DNAPL). The high temperatures may have an adverse effect on the stability of microbial populations in the subsurface. To study the microbial ecology associated with resistive heating, lab-scale experiments were performed in insulated Lexan® boxes (0.5 m H x 0.5 m W X 0.1 m H) containing soil from the Piedmont region of North Carolina (Medium sand). Sterile water, organic media, and inorganic media additions were made after the heating and cooling. Microbial activity in soils before and after heating was obtained by means of plate counts and Acridine Orange Direct counts (AODC) and Phospholipid Fatty Acid Analysis (PLFA). It was observed that after resistive heating the microbial counts diminish to small numbers. After nutrient addition and a couple of days of growth, population numbers begin recovering with the population consisting of more gram positive microbes than in the initial soil. The heating and cooling temperature profiles generated during the experiments were compared to those generated from mathematical heat transfer models. Single-phase models were set up in a 2D grid with porous media properties and appropriate boundary conditions. Sensitivity of the single-phase model to different values of soil properties and fluid properties was analyzed for adiabatic and non-adiabatic cases. The results indicate that by using typical soil properties and values of the convective heat transfer coefficient, agreement can be reached between the experimental and theoretical temperatures.

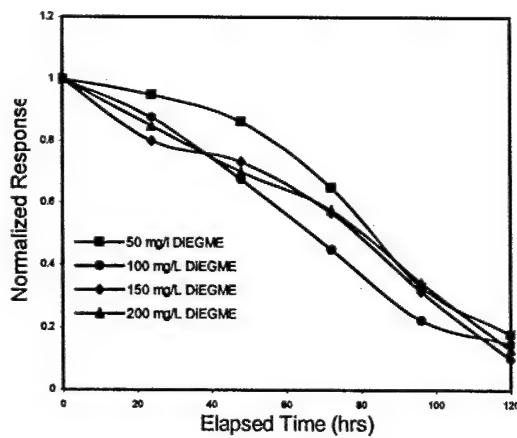
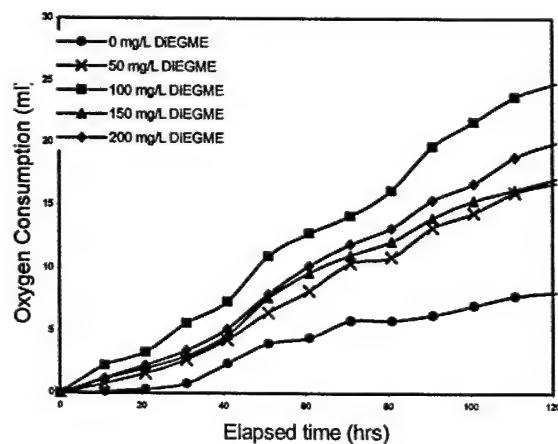


**Project Title:** Biodegradation of an Aviation Fuel System Containing Icing Inhibitors

**Investigator(s):** Keith Schimmel

**Student(s):** Bhama Bhat, Pavithra Jayaraman

**Summary:** The current fuel system icing inhibitor (FSII) used for commercial and military aircraft is diethylene glycol monomethyl ether (DiEGME). Fuel deicing agents are mandatory in military fuels and optional in commercial fuels, but the biodegradation behavior of DiEGME is unknown. Standard 5-day BOD tests were conducted for DiEGME in an aerobic respirometer with substrate concentrations of 2, 5, 10, 50, 100, 150 and 200 mg/L. Pure cultures of the bacteria OR 2A Awd, isolated from glycol contaminated soil samples from Alaska were used in this study. The cell growth and substrate concentration were monitored by extracting samples periodically and analyzing them using a spectrophotometer and gas chromatograph/mass spectrometer. Results obtained indicate that DiEGME is degraded by the bacterial strain used. Reproducible oxygen consumption patterns are observed in the respirometer data, steady growth of microorganisms and almost 90% substrate degradation is observed in most cases. The degradation of DiEGME, also studied in the presence of a second fuel additive, the antioxidant butylated hydroxy toluene (BHT), was found to be significantly inhibited. Degradation studies were also performed on a newly synthesized FSII, M1. This compound did not show significant degradation with the bacterial strain used.

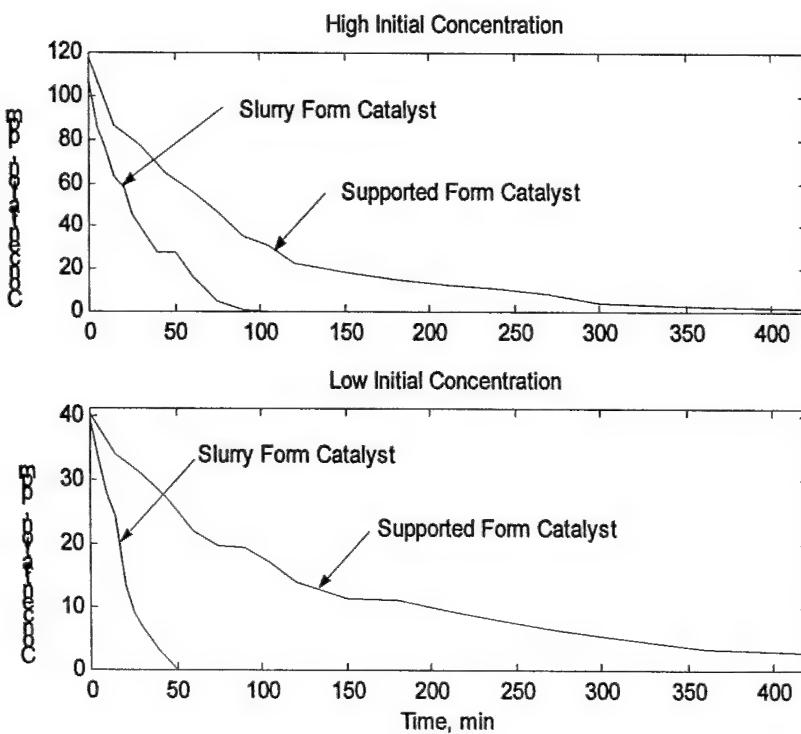


**Project Title:** Supported TiO<sub>2</sub> Catalyst for Photocatalytic Detoxification

**Investigator(s):** Vinayak N. Kabadi

**Student(s):** Shahnaj Begum, David Williams

**Summary:** A vast amount of work is available in the literature on the conditions and mechanisms governing TiO<sub>2</sub> photocatalytic reactions, but a feasible technology for continuous photocatalytic water treatment is still not available. TiO<sub>2</sub> is generally used in the form of a slurry, and although it is very effective in degradation of common organic chemicals, it poses some problems in having to be filtered out of the treated water. Supported form of catalyst is an alternative to avoid any post-treatment. In this study, we have developed a supported form of catalyst which consists of a thin film of TiO<sub>2</sub> deposited on the surface of polypropylene beads. The effectiveness of the catalyst was demonstrated by successful degradation of trichloroethylene (TCE) in a pot reactor. The degradation curves are shown in the two figures. Degradation curves for the catalyst in the slurry form are also shown. Langmuir-Hinshelwood kinetics was used to model the degradation rates, and the kinetic parameters were computed. Usage of the catalyst for continuous purification of water was demonstrated in a continuous flow packed bed reactor.



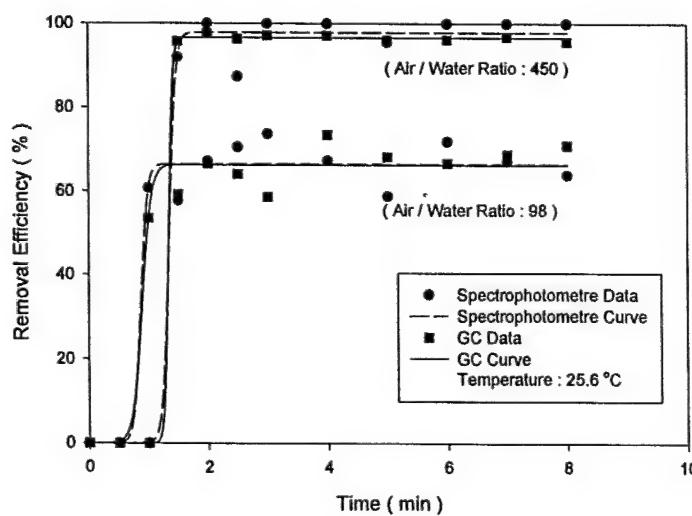
**Project Title:** Low-Profile Gas Stripping of Organic Pollutants and Destruction by Gas-Phase Photolysis.

**Investigator:** Yusuf G. Adewuyi

**Students:** Vicky Harrison, Riyad A. Jadalla, Collins Appaw

**Summary:** Contamination of soil and groundwater is a serious health and environmental problem. Contamination sources include manufacturing plants, petroleum refineries, fuel and chemical storage facilities, gas service stations, underground storage tank leaks, poor disposal practices, chemical wastes from agricultural practices, and accidental spills of contaminants. The majority of the contaminants are volatile organic compounds (VOCs). VOCs commonly found in water include BTX, naphthalene, acetone, and a wide range of chlorinated hydrocarbons such as TCE, tetrachloroethane and trichloroethane. The objectives of this project were to determine the feasibility of effectively decontaminating polluted water by coupling air stripping (using Shallow-tray, low-profile air stripper) with UV-catalyzed photolysis directly in the gas phase (using xenon flashlamps and UV pulsed lamps). The first phase of this project sought to determine the capabilities and limitations of tray-type (Shallow TrayTM) air-stripping technology in remediating water contaminated with volatile organic compounds. We have successfully completed work on the stripping of benzene, toluene, ethylbenzene, and xylenes (BTEX), trichloroethylene (TCE), methyl tert-butyl ether (MTBE) and acetone. Results were obtained by sampling and analyzing the inlet and outlet water streams from the stripper using both a UV/VIS spectrophotometer (DU 750, Beckman) set at wavelength of 210-190 nm and GC (HP 6890). The results using both analytical techniques agreed perfectly. The second phase of this project – photolysis, requires the use of GC/MS on-line with the xenon flashlamp attached to the stripper. Unfortunately, due budget limitations we could not purchase a new mass spectrometer (MS) and the one MS available for Fast Center researchers could not be disconnected from existing GC for use online with the stripper. As a result, the photolysis aspect of this project was put on hold.

Comparison of GC and Spectrophotometric Analysis for MTBE  
( Inlet Concentration : 727 - 824 ppm )

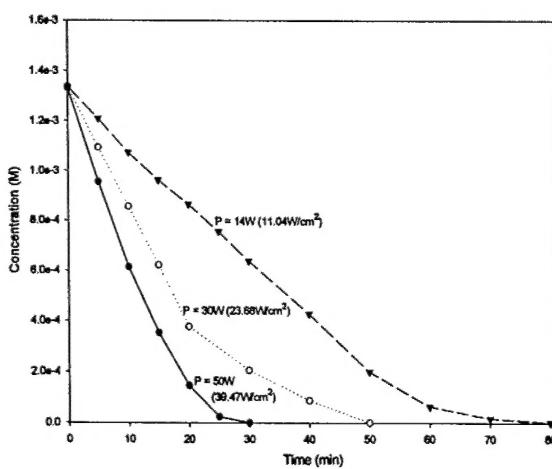


**Project Title:** Sonochemical Degradation of Aqueous Organic and Inorganic Pollutants

**Investigator:** Yusuf G. Adewuyi

**Students:** Collins Appaw, Samuel Owusu, Babatunde Oyenekan

**Summary:** Sonochemical engineering is a field involving the application of sonic and ultrasonic waves to chemical processing. The application of sonochemistry to environmental remediation is a developing technology and an understanding of the fundamentals and engineering aspects involved are not fully understood. Sonochemistry enhances or promotes chemical reactions and mass transfer. Application of this novel means of reaction in environmental remediation is a rapidly growing area. Sonochemical oxidation has been investigated as an environmentally benign process for removing halogenated and non-halogenated organic species from wastewater streams. This project focuses on the sonochemical destruction of organic and inorganic compounds in aqueous solutions. Several sonochemical batch and flow reactors (e.g., bubble column, stirred cell) were designed and constructed. The kinetics of the sonochemical degradation of aqueous carbon disulfide was studied in a batch reactor at 20 kHz and the effects of process parameters (e.g. concentration, temperature, ultrasonic intensity) investigated. The concentrations of unbuffered  $\text{CS}_2$  solutions used were  $6.4\text{--}7.0 \times 10^{-4}\text{M}$ ,  $10.5 \times 10^{-4}\text{M}$  and  $13.2\text{--}13.6 \times 10^{-4}\text{M}$ . The intensities were varied from 14–50W and the temperatures from 20–50°C. The reaction rate was found to be zero order in the temperature range studied. The rate constant for the degradation at 20°C, 14W and in air was  $2.27 \times 10^{-5} \text{ min}^{-1}$ . At the same initial concentrations and temperature, and in the presence of air, the degradation rate of  $\text{CS}_2$  at 50 W ( $39.47 \text{ W/m}^2$ ) is more than two times that at 14 W ( $11.04 \text{ W/m}^2$ ). The rate constant for the degradation at 20°C, 14W and in air was  $2.27 \times 10^{-5} \text{ min}^{-1}$ . At the same initial concentrations and temperature, and in the presence of air, the degradation rate of  $\text{CS}_2$  at 50 W ( $39.47 \text{ W/m}^2$ ) is more than two times that at 14 W ( $11.04 \text{ W/m}^2$ ). The rate of sonochemical degradation of  $\text{CS}_2$  in the presence of the different gases was in the order of He > Air > Ar; the rate with helium was found to be about three times of argon. We also evaluated the kinetics and mechanisms of reactions, products of reactions and yields, and the effects of solution pH changes. We have also demonstrated that ultrasonic irradiation induces the absorption and oxidation of nitric oxide. We conducted experiments in a bubble column operated as batch or continuous reactor at 20 kHz and investigated the effects of process parameters (e.g. concentration, pH, temperature, ultrasonic intensity, irradiation medium, etc.). We also evaluated the influence solution ionic strength using NaCl and presence of  $\text{SO}_2$  on the sonochemical oxidation of  $\text{NO}_x$ .

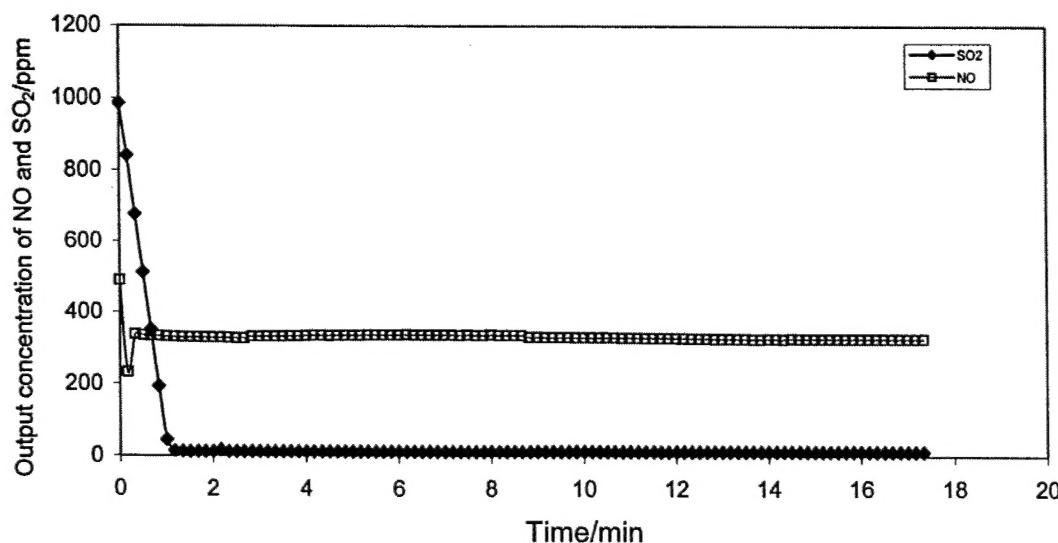


**Project Title:** Reactive Mass Transfer for Air Pollution Abatement

**Investigator(s):** Yusuf G. Adewuyi

**Students:** Samuel Owusu, Babatunde Oyenekan

**Summary:** The emission of  $\text{NO}_x$  and  $\text{SO}_x$  into the atmosphere is a major environmental concern because of their detrimental effects (e.g. acid rain) on mankind and its ecosystems. Scrubbing the gases with an aqueous alkaline slurry (or liquid) is a widely used treatment process and removes over 90% of the  $\text{SO}_2$  and particulate. However, nitric oxide ( $\text{NO}$ ) has posed a persistent problem for industry in that it cannot be easily removed from incinerators and boilers by scrubbing as are nitrogen dioxide ( $\text{NO}_2$ ) and sulfur dioxide ( $\text{SO}_2$ ) due to its low solubility in water. However, scrubbing promises to be less expensive than competing post-combustion methods for  $\text{NO}_x$  removal such as selective catalytic reduction (SCR) and thermal  $\text{NO}_x$  removal. The goal of this project is to develop an innovative and cost-effective aqueous scrubber for the simultaneous removal and destruction of oxides of nitrogen and sulfur, and other air toxic emissions such as volatile organic compounds (VOCs). We have completed work on the aqueous absorption and kinetics of oxidation of nitrogen oxides ( $\text{NO}_x$ ) and  $\text{SO}_2$  by OXONE in a bubble column operated as batch or continuous reactor at various process conditions. OXONE is a triple salt of potassium ( $2\text{KHSO}_5 \cdot \text{KHSO}_4 \cdot \text{K}_2\text{SO}_4$ ) and is a strong oxidant that may be regarded as a mono-substituted derivative of hydrogen peroxide. However, it has an oxidation potential greater than that of hydrogen peroxide ( $E_{\text{HSO}_5^{\cdot}/\text{HSO}_4^-} = 1.82 \text{ eV}$  compared to  $E_{\text{H}_2\text{O}_2/\text{H}_2\text{O}} = 1.77 \text{ eV}$ ). We have investigated the influence of different variables such as temperature, gas stream flow rate (or residence time), concentration of oxone, solution pH, feed concentration of NO and the presence of  $\text{SO}_2$  on the rate of NO removal and oxidation. With an aqueous concentration of 0.02M OXONE, fractional conversion of NO (feed concentration of 500-1000 ppm and flow rate of 0.1-1.0 L/min) was found to range from 60-86% at room temperature ( $22^\circ\text{C}$ ) with the optimal removal and oxidation in the pH range 6.5-8.5. The fractional conversion for  $\text{SO}_2$  was over 98% (feed concentration 1000-5000 ppm) for all experimental runs. We also completed studies on the simultaneous and individual absorption of NO,  $\text{SO}_2$  into aqueous solutions of  $\text{NaClO}_2$ .

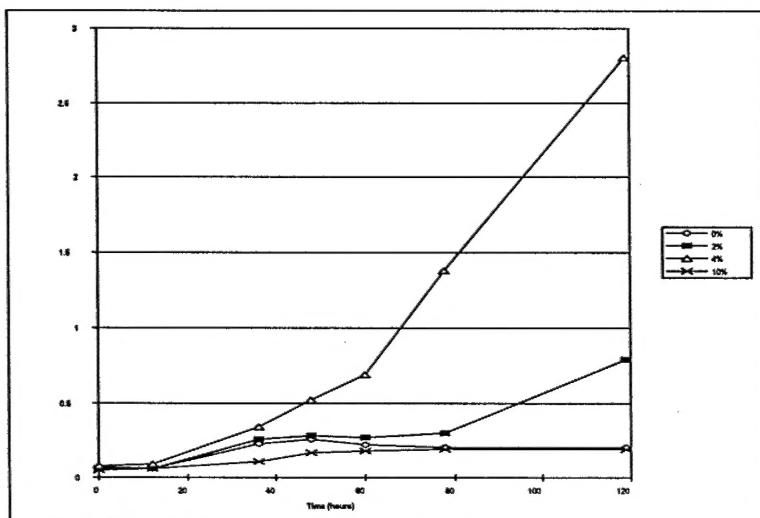


**Project Title: Isolation and Growth of Glycol Degrading Bacteria**

**Investigator(s):** Thomas Jordan

**Student(s):** Dexter McQueen

**Abstract:** Alaskan soil contaminated with propylene and triethylene glycol and samples from the North Carolina A&T Hog Lagoon were collected and used as a source of propylene and triethylene glycol degrading bacteria. Alaskan soil was used to isolate bacteria with a tolerance for high concentration of deicing agents, and to compare them with bacteria from a temperate climate that had not been exposed to the chemicals. We have isolated six strains of propylene and triethylene glycol degrading bacteria. All of the strains were gram negative. The strains were identified as Xanthomonas maltophilia (OR-2AB-wd), Alcaligenes faecalis (OR-2AA-wf) and Alcaligenes faecalis (HTEG-w), Pseudomonas diminuta (TEG-OR-SB-wl) and Serratia fonticola (HPGM-w) and Serratia fonticola (OR-2AA-wf). The bacteria were grown aerobically at 30°C in media containing 2%, 4%, and 10% by volume of either propylene or triethylene glycol in defined media. All of the strains grew well at concentrations of 2% and 4%, but all except Xanthomonas maltophilia (OR-2AB-wd), were inhibited and failed to grow in media containing 10% glycol. The unacclimated bacteria from the hog lagoon grew as well as the acclimated Alaskan strains. Bacterial growth was stimulated by supplementing the propylene glycol medium with Peptone Yeast Extract (PYE) or glucose and the triethylene glycol medium with glucose. This suggests that the use of these bacteria to degrade deicer waste may be stimulated by supplementation with peptone yeast extract or glucose.



**Project Title:** Molecular Dynamics Simulations of Phenomena at the Air-Water and Oil-Water Interfaces

**Investigator(s):** Vinayak N. Kabadi

**Student(s):** Parag S. Adhangale

**Summary:** A number of processes of environmental significance occur at the air-water and the oil-water interfaces. The concentrations of the pollutant materials in the air, water, or land many times are functions of equilibria and kinetics of these interfacial processes. The literature is full of numerous experimental and theoretical studies of such phenomena. Only in recent times, attempts are being made to apply the technique of molecular simulations and modeling to liquid-liquid and gas-liquid interfaces. In this project, our objective is to use molecular dynamics computer simulations to simulate stable oil-water and air-water interfaces, and then to study the structural, dynamic and transport properties of simple polar organic molecules at the two interfaces. So far we have developed the computer code for the two interfacial simulations. We have successfully simulated a stable oil-water interface, but have not yet been successful in getting a stable air-water interface. The main problem with our current method is the accounting for the electrostatic interactions of water molecules. We have simply used a long-range coulombic potential with spherical truncation. Using Ewald summations to represent electrostatic interactions of water molecules would be more accurate, and would be expected to give more realistic results. Attempts to introduce this complex process of Ewald summations in our code are currently under way. Once this process is completed, the two simulated interfaces will be ready for environmental applications.

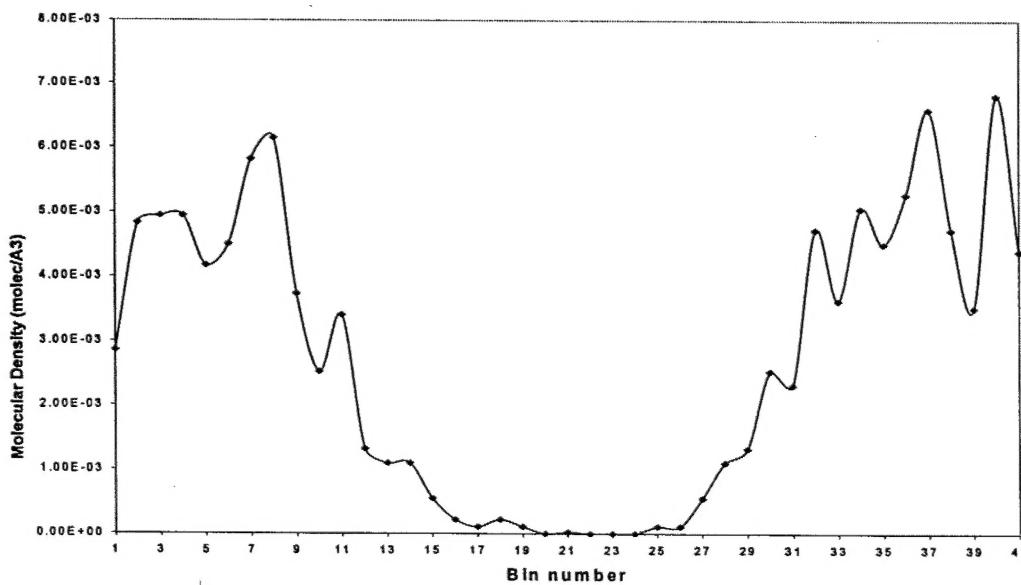


Figure: Density of water molecules across the air-water interface